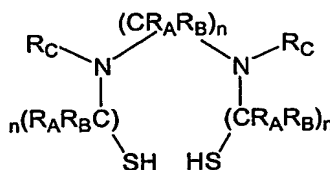


What is claimed is

1. A compound capable of binding a metal ion, the compound according to the formula:



wherein:

$\text{R}_A$  is independently chosen at each occurrence of  $\text{R}_A$  from the group consisting of hydrogen, lower alkyl having 1 to about 4 carbon atoms, alkyl ester groups having about 2 to about 8 carbon atoms, aryl ester groups having about 7 to about 18 carbon atoms, alkyl amide groups having about 2 to about 8 carbon atoms, aryl amide groups having about 7 to about 18 carbon atoms, di(alkyl)aminoalkyl groups where each alkyl group has 1 to about 4 carbon atoms, and  $-\text{XNR}_1\text{R}_2$ ;

$\text{R}_B$  is hydrogen or a lower alkyl group having from 1 to about 6 carbon atoms for each occurrence of  $\text{R}_B$ ; or

$-(\text{C R}_A \text{R}_B)-$  taken in combination is  $-(\text{C}=\text{O})-$  such that there are zero or one  $-(\text{C}=\text{O})-$  groups;

$\text{R}_C$  is independently selected at each occurrence of  $\text{R}_C$  from the group consisting of hydrogen, lower alkyl groups having 1 to about 8 carbon atoms, alkoxyalkyl group having from 2 to about 8 carbon atoms, alkyl ester or aryl ester groups having about 2 to about 8 carbon atoms, alkyl amide or aryl amide groups having about 2 to 8 carbon atoms, di(alkyl)aminoalkyl groups where each alkyl group has 1 to about 4 carbon atoms, and  $-\text{XNR}_1\text{R}_2$ ;

$\text{X}$  is a linking group comprising a backbone chain having 1 to about 8 atoms, the backbone chain can optionally include ester, amide, ether or thioether linkages in the backbone chain; and

$\text{R}_1$  and  $\text{R}_2$  each are independently selected unsubstituted alkyl groups having from 1 to about 8 carbon atoms, alkoxyalkyl group having from 2 to about 8 carbon atoms, and substituted alkyl or alkoxyalkyl groups having from 1 to about 8 carbon atoms which are substituted with one or more groups selected from optionally substituted aryl, optionally

substituted cycloalkyl, optionally substituted heteroalicyclic, and optionally substituted heteroaryl, wherein at least one of  $R_1$  or  $R_2$  is a substituted alkyl or alkyloxy group;

$n$  is either 2 or 3 and is independently chosen at each occurrence of  $n$ ; and

at least one occurrence of  $R_A$  or  $R_C$  in Formula I is chosen to be  $-XNR_1R_2$ ,

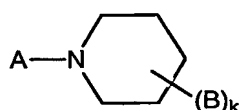
5 where the metal complex resulting from the binding of the compound to the metal ion is either neutral or cationic.

2. The compound of claim 1, wherein  $X$  is an optionally substituted  $C_{2-8}$ alkylene group,  $R_1$  is  $C_{1-6}$ alkyl group and  $R_2$  is an optionally substituted (aryl) $C_{1-4}$ alkyl or an optionally substituted (heteroaryl) $C_{1-4}$ alkyl.

3. The compound of claim 1 or claim 2, wherein the compound is capable of binding a metal ion selected from the group consisting of technetium, rhenium, yttrium, copper, gallium, indium, bismuth, platinum and rhodium.

4. The compound of any one of claims 1-3, wherein the compound is capable of binding technetium or rhenium.

5. A compound capable of binding a metal ion, the compound according to the formula:



wherein

25 A is selected from the group consisting of optionally substituted alkyl, optionally substituted alkenyl, optionally substituted alkynyl, optionally substituted aryl, optionally substituted aralkyl, optionally substituted cycloalkyl, optionally substituted heteroalicyclic, optionally substituted heteroaralkyl, optionally substituted heteroaryl, and  $-X-Y$ ;

30 B is independently selected at each occurrence of B from the group consisting of optionally substituted alkyl, optionally substituted alkenyl, optionally substituted alkynyl, hydroxy, optionally substituted alkoxy, halogen, hydroxy, optionally substituted alkoxyalkyl,

optionally substituted amino, optionally substituted mono and dialkyl amino, optionally substituted aryl, optionally substituted aralkyl, optionally substituted cycloalkyl, optionally substituted heteroalicyclic, optionally substituted heteroaralkyl, optionally substituted heteroaryl, and -X-Y;

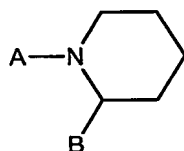
5 X is a linking group comprising a backbone chain having 1 to about 8 atoms, the backbone chain can optionally include ester, amide, ether or thioether linkages in the backbone chain;

k is an integer from about 1 to about 3; and

Y is a group capable of chelating to at least one metal ion,

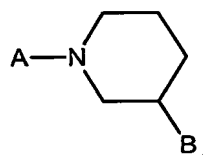
10 wherein at least one of A or B is chosen to be -X-Y.

6. A compound of claim 5 according to the formula:



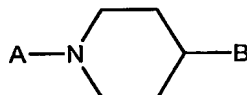
15

7. A compound of claim 5 according to the formula:



8. A compound of claim 5 according to the formula:

20

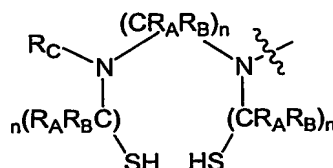


9. The compound of claim 5, wherein Y comprises two or more N, S, or P atoms which are capable of chelating the metal ion.

25

10. The compound of claim 5, wherein Y is a tridentate or tetradentate chelate having three or more heteroatoms selected from N, P, or S atoms, which is capable of binding the metal ion.

5 11. The compound of claim 5, wherein Y is a group of the formula:



wherein:

$R_A$  is independently chosen at each occurrence of  $R_A$  from the group consisting of  
 10 hydrogen, lower alkyl having 1 to about 4 carbon atoms, alkyl ester groups having about 2 to about 8 carbon atoms, aryl ester groups having about 7 to about 18 carbon atoms, alkyl amide groups having about 2 to about 8 carbon atoms, aryl amide groups having about 7 to about 18 carbon atoms, di(alkyl)aminoalkyl groups where each alkyl group has 1 to about 4 carbon atoms, and  $-XNR_1R_2$ ;

15  $R_B$  is hydrogen or lower alkyl having from about 1 to about 6 carbon atoms for each occurrence of  $R_B$ ; or

$-(CR_AR_B)-$  taken in combination is  $-(C=O)-$  such that there are zero or one  $-(C=O)-$  groups;

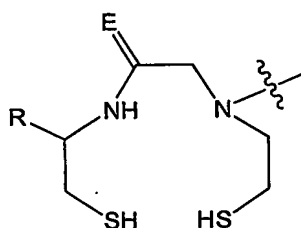
$R_C$  is selected from the group consisting of hydrogen, lower alkyl groups having 1 to  
 20 about 8 carbon atoms, alkoxyalkyl group having from 2 to about 8 carbon atoms, alkyl ester or aryl ester groups having about 2 to about 8 carbon atoms, alkyl amide or aryl amide groups having about 2 to 8 carbon atoms, di(alkyl)aminoalkyl groups where each alkyl group has 1 to about 4 carbon atoms, and  $-XNR_1R_2$ ;

$X$  is a linking group comprising a backbone chain having 1 to about 8 atoms, the  
 25 backbone chain can optionally include ester, amide, ether or thioether linkages in the backbone chain ; and

$R_1$  and  $R_2$  each are independently selected unsubstituted alkyl groups having from 1 to about 8 carbon atoms, alkoxyalkyl group having from 2 to about 8 carbon atoms, and substituted alkyl or alkoxyalkyl groups having from 1 to about 8 carbon atoms which are

substituted with one or more groups selected from optionally substituted aryl, optionally substituted cycloalkyl, optionally substituted heteroalicyclic, optionally substituted heteroaryl;  
 n is either 2 or 3 and is independently chosen at each occurrence of n.

- 5            12. The compound of claim 11, wherein the group Y is selected from groups according to the formula:



wherein

- 10            R is selected from hydrogen, C(O)O(R<sub>3</sub>), or C(O)NH(R<sub>3</sub>);

R<sub>3</sub> represents hydrogen, optionally substituted alkyl, optionally substituted alkenyl, optionally substituted alkynyl, optionally substituted aryl, optionally substituted aralkyl, and optionally substituted cycloalkyl;

E represents an oxo group or two hydrogen atoms.

15

13. The compound of claim 5, wherein X is selected from the group consisting of  $-(CH_2)_m-C(O)NH-$  and  $\alpha,\omega$ -alkylene groups wherein the alkylene group has between about 1 and about 10 carbon atoms and between 0 and about 3 oxygen or sulfur atoms in the alkylene chain;

20

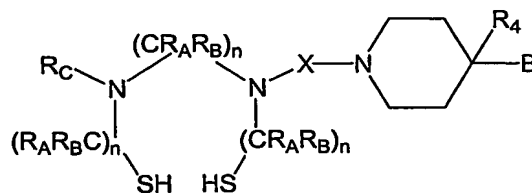
m is an integer of from about 1 to about 5.

14. The compound of claim 5, wherein the compound is capable of binding a metal ion selected from the group consisting of technetium, rhenium, yttrium, copper, gallium, indium, bismuth, platinum and rhodium.

25

15. The compound of claim 5, wherein the compound is capable of binding technetium or rhenium.

16. A compound capable of binding a metal ion, the compound according to the formula:



5 wherein:

B is selected from the group consisting of optionally substituted alkyl, optionally substituted alkenyl, optionally substituted alkynyl, hydroxy, optionally substituted alkoxy, optionally substituted alkoxyalkyl, optionally substituted amino, optionally substituted mono and dialkyl amino, halogen, optionally substituted aryl, optionally substituted aralkyl, optionally substituted cycloalkyl, optionally substituted heteroalicyclic, optionally substituted heteroaralkyl, optionally substituted heteroaryl, and -X-Y;

R<sub>4</sub> is hydrogen, hydroxy, halogen, optionally substituted alkyl groups having from 1 to about 6 carbon atoms, optionally substituted alkoxy groups having from 1 to about 6 carbon atoms, or

15 R<sub>4</sub> and B taken in combination form an optionally substituted heterocyclic group having 5 or 12 ring atoms and one or two N, O, or S atoms and 1 or 2 fused rings;

R<sub>A</sub> is independently chosen at each occurrence of R<sub>A</sub> from the group consisting of hydrogen, lower alkyl having 1 to about 4 carbon atoms, alkyl ester groups having about 2 to about 8 carbon atoms, aryl ester groups having about 7 to about 18 carbon atoms, alkyl amide groups having about 2 to about 8 carbon atoms, aryl amide groups having about 7 to about 18 carbon atoms, di(alkyl)aminoalkyl groups where each alkyl group has 1 to about 4 carbon atoms, and -XNR<sub>1</sub>R<sub>2</sub>;

R<sub>B</sub> is hydrogen or lower alkyl having from 1 to about 4 carbon atoms for each occurrence of R<sub>B</sub>; or

25 -(C R<sub>A</sub> R<sub>B</sub>)- taken in combination is -(C=O)- such that there are zero or one -(C=O)- groups;

R<sub>C</sub> is selected from the group consisting of hydrogen, lower alkyl groups having 1 to about 8 carbon atoms, alkoxyalkyl group having from 2 to about 8 carbon atoms, alkyl ester or aryl ester groups having about 2 to about 8 carbon atoms, alkyl amide or aryl amide groups

having about 2 to 8 carbon atoms, di(alkyl)aminoalkyl groups where each alkyl group has 1 to about 4 carbon atoms, and  $-XNR_1R_2$ ;

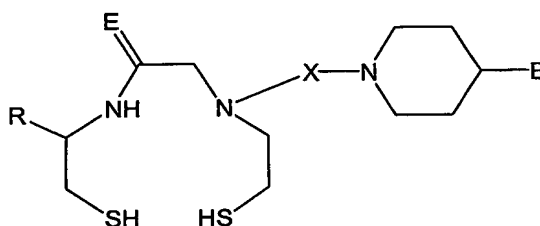
Y is a group capable of chelating to at least one metal ion;

X is a linking group comprising a backbone chain having 1 to about 8 atoms, the  
 5 backbone chain can optionally include ester, amide, ether or thioether linkages in the backbone chain ;

$R_1$  and  $R_2$  each are independently selected unsubstituted alkyl groups having from 1 to about 8 carbon atoms, alkoxyalkyl group having from 2 to about 8 carbon atoms, and substituted alkyl or alkoxyalkyl groups having from 1 to about 8 carbon atoms which are  
 10 substituted with one or more groups selected from optionally substituted aryl, optionally substituted cycloalkyl, optionally substituted heteroalicyclic, and optionally substituted heteroaryl; and

n is either 2 or 3 and is independently chosen at each occurrence of n.

15 17. The compound of claim 16, the compound according to the formula:



wherein:

B is selected from the group consisting of optionally substituted alkyl, optionally  
 20 substituted alkenyl, optionally substituted alkynyl, hydroxy, optionally substituted alkoxy, optionally substituted alkoxyalkyl, optionally substituted amino, optionally substituted mono and dialkyl amino, halogen, optionally substituted aryl, optionally substituted aralkyl, optionally substituted cycloalkyl, optionally substituted heteroalicyclic, optionally substituted heteroaralkyl, optionally substituted heteroaryl, and  $-X-Y$ ;

25 Y is a group capable of chelating to at least one metal ion;

R is selected from hydrogen,  $C(O)O(R_3)$ , or  $C(O)NH(R_3)$ ;

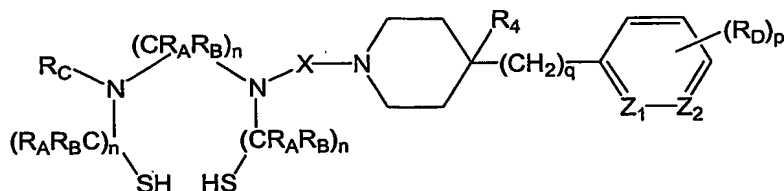
$R_3$  represents hydrogen, optionally substituted alkyl, optionally substituted alkenyl, optionally substituted alkynyl, optionally substituted aryl, optionally substituted aralkyl, and optionally substituted cycloalkyl;

E represents an oxo group or two hydrogen atoms; and

X is a linking group comprising a backbone chain having 1 to about 8 atoms, the backbone chain can optionally include ester, amide, ether or thioether linkages in the backbone chain.

5

18. A compound capable of binding a metal ion, the compound according to the formula:



10 wherein:

$R_D$  is independently selected at each occurrence from the group consisting of optionally substituted alkyl, optionally substituted alkenyl, optionally substituted alkynyl, hydroxy, amino, halogen, cyano, nitro, optionally substituted alkoxy, optionally substituted alkoxyalkyl, optionally substituted mono and dialkyl amino, optionally substituted aryl, optionally substituted heteroaryl, optionally substituted cycloalkyl, optionally substituted heteroalicyclic groups;

15

$R_4$  is hydrogen, hydroxy, halogen, optionally substituted alkyl groups having from 1 to about 6 carbon atoms, optionally substituted alkoxy groups having from 1 to about 6 carbon atoms, or

20

$Z_1$  and  $Z_2$  are independently selected from CH,  $CR_D$ , and N;

$p$  is selected from integers between about 0 and about 5;

$q$  is selected from integers between about 0 and about 10;

$R_A$  is independently chosen at each occurrence of  $R_A$  from the group consisting of hydrogen, lower alkyl having 1 to about 4 carbon atoms, alkyl ester groups having about 2 to about 8 carbon atoms, aryl ester groups having about 7 to about 18 carbon atoms, alkyl amide groups having about 2 to about 8 carbon atoms, aryl amide groups having about 7 to about 18 carbon atoms, di(alkyl)aminoalkyl groups where each alkyl group has 1 to about 4 carbon atoms, and  $-XNR_1R_2$ ;

25

$R_B$  is hydrogen or lower alkyl having from about 1 to about 4 carbon atoms for each occurrence of  $R_B$ ; or

30



$-(CR_A R_B)-$  taken in combination is  $-(C=O)-$  such that there are zero or one  $-(C=O)-$  groups;

$R_C$  is selected from the group consisting of hydrogen, lower alkyl groups having 1 to about 8 carbon atoms, alkoxyalkyl groups having from 2 to 8 carbon atoms, alkyl ester or aryl ester groups having about 2 to about 8 carbon atoms, alkyl amide or aryl amide groups having about 2 to 8 carbon atoms, di(alkyl)aminoalkyl groups where each alkyl group has 1 to about 4 carbon atoms, and  $-XNR_1R_2$ ;

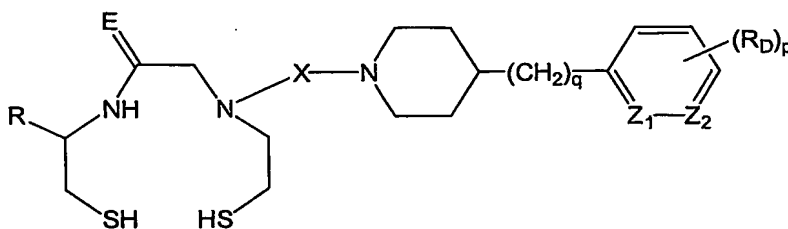
$Y$  is a group capable of chelating to at least one metal ion;

$X$  is a linking group comprising a backbone chain having 1 to about 8 atoms, the backbone chain can optionally include ester, amide, ether or thioether linkages in the backbone chain ;

$R_1$  and  $R_2$  each are independently selected unsubstituted alkyl groups having from 1 to about 8 carbon atoms, alkoxyalkyl group having from 2 to about 8 carbon atoms, and substituted alkyl or alkoxyalkyl groups having from 1 to about 8 carbon atoms which are substituted with one or more groups selected from optionally substituted aryl, optionally substituted cycloalkyl, optionally substituted heteroalicyclic, and optionally substituted heteroaryl; and

$n$  is either 2 or 3 and is independently chosen at each occurrence of  $n$ .

19. The compound of claim 18, the compound according to the formula:



wherein:

$R_D$  is independently selected at each occurrence from the group consisting of optionally substituted alkyl, optionally substituted alkenyl, optionally substituted alkynyl, hydroxy, amino, halogen, cyano, nitro, optionally substituted alkoxy, optionally substituted alkoxyalkyl, optionally substituted mono and dialkyl amino, optionally substituted aryl, optionally substituted heteroaryl, optionally substituted cycloalkyl, and optionally substituted heteroalicyclic groups;

$Z_1$  and  $Z_2$  are independently selected from CH,  $CR_D$ , and N;

$p$  is selected from integers between about 0 and about 5;

$q$  is selected from integers between about 0 and about 10;

$R$  is selected from hydrogen,  $C(O)O(R_3)$ , or  $C(O)NH(R_3)$ ;

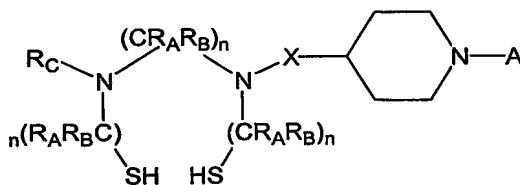
5  $R_3$  represents hydrogen, optionally substituted alkyl, optionally substituted alkenyl, optionally substituted alkynyl, optionally substituted aryl, optionally substituted aralkyl, and optionally substituted cycloalkyl;

$E$  represents an oxo group or two hydrogen atoms; and

10  $X$  is a linking group comprising a backbone chain having 1 to about 8 atoms, the backbone chain can optionally include ester, amide, ether or thioether linkages in the backbone chain.

20. A compound capable of binding a metal ion, the compound according to the formula:

15



wherein:

20  $A$  is selected from the group consisting of optionally substituted alkyl, optionally substituted alkenyl, optionally substituted alkynyl, optionally substituted aryl, optionally substituted aralkyl, optionally substituted cycloalkyl, optionally substituted heteroalicyclic, optionally substituted heteroaralkyl, optionally substituted heteroaryl, and  $-X-Y$ ;

25  $R_A$  is independently chosen at each occurrence of  $R_A$  from the group consisting of hydrogen, lower alkyl having 1 to about 4 carbon atoms, alkyl ester groups having about 2 to about 8 carbon atoms, aryl ester groups having about 7 to about 18 carbon atoms, alkyl amide groups having about 2 to about 8 carbon atoms, aryl amide groups having about 7 to about 18 carbon atoms, di(alkyl)aminoalkyl groups where each alkyl group has 1 to about 4 carbon atoms, and  $-XNR_1R_2$ ;

$R_B$  is hydrogen or lower alkyl having from about 1 to about 4 carbon atoms for each occurrence of  $R_B$ ; or

-(CR<sub>A</sub>R<sub>B</sub>)- taken in combination is -(C=O)- such that there are zero or one -(C=O)- groups;

R<sub>C</sub> is selected from the group consisting of hydrogen, lower alkyl groups having 1 to about 8 carbon atoms, alkoxyalkyl groups having from 2 to 8 carbon atoms, alkyl ester or aryl ester groups having about 2 to about 8 carbon atoms, alkyl amide or aryl amide groups having about 2 to 8 carbon atoms, di(alkyl)aminoalkyl groups where each alkyl group has 1 to about 4 carbon atoms, and -XNR<sub>1</sub>R<sub>2</sub>;

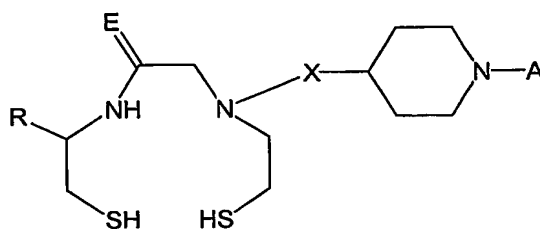
Y is a group capable of chelating to at least one metal ion;

X is a linking group comprising a backbone chain having 1 to about 8 atoms, the backbone chain can optionally include ester, amide, ether or thioether linkages in the backbone chain ;

R<sub>1</sub> and R<sub>2</sub> each are independently selected unsubstituted alkyl groups having from 1 to about 8 carbon atoms, alkoxyalkyl group having from 2 to about 8 carbon atoms, and substituted alkyl or alkoxyalkyl groups having from 1 to about 8 carbon atoms which are substituted with one or more groups selected from optionally substituted aryl, optionally substituted cycloalkyl, optionally substituted heteroalicyclic, and optionally substituted heteroaryl; and

n is either 2 or 3 and is independently chosen at each occurrence of n.

21. The compound of claim 20, the compound according to the formula:



wherein:

A is selected from the group consisting of optionally substituted alkyl, optionally substituted alkenyl, optionally substituted alkynyl, optionally substituted aryl, optionally substituted aralkyl, optionally substituted cycloalkyl, optionally substituted heteroalicyclic, optionally substituted heteroaralkyl, optionally substituted heteroaryl, and -X-Y;

R is selected from hydrogen, C(O)O(R<sub>3</sub>), or C(O)NH(R<sub>3</sub>);

$R_3$  represents hydrogen, optionally substituted alkyl, optionally substituted alkenyl, optionally substituted alkynyl, optionally substituted aryl, optionally substituted aralkyl, and optionally substituted cycloalkyl;

E represents an oxo group or two hydrogen atoms; and

- 5 X is a linking group comprising a backbone chain having 1 to about 8 atoms, the backbone chain can optionally include ester, amide, ether or thioether linkages in the backbone chain.

22. The compound of any one of claims 1 through 21, wherein the compound is capable of binding to one or more proteins and/or receptors or neuroreceptors, such as  
 10 serotonin receptors,  $\alpha$  receptors,  $\sigma$  receptors, calcium channel receptors, emopamil binding proteins, adrenergic receptors, adrenoceptors receptors, dopamine receptors, sigma receptors and any subtype or subclass thereof.

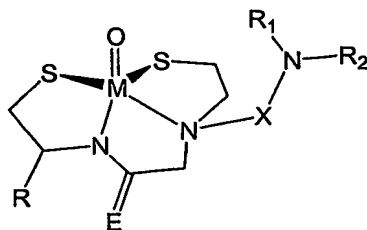
23. The compound of claim 22, wherein the receptor(s) are selected from  $5HT_{1A}$ ,  
 15  $\sigma_1$ ,  $\sigma_2$ ,  $\alpha_1$ ,  $Ca^{+2}$  channel receptors, EBP or a combination thereof.

24. A neutral or cationic complex comprising a metal ion and a compound according to any one of claims 1 through 21.

- 20 25. The neutral or cationic complex of claim 24, wherein the metal ion is one or more isotopes of a metal selected from the group consisting of technetium, rhenium, yttrium, copper, gallium, indium, bismuth, platinum and rhodium.

26. A neutral or cationic complex of claim 24, wherein the metal ion is selected  
 25 from one or more isotopes of technetium or one or more isotopes of rhenium.

27. A complex of claim 24, wherein the complex is of the formula:



wherein

M is one or more isotopes of technetium or rhenium;

X is a linking group comprising a backbone chain having 1 to about 8 atoms, the backbone chain can optionally include ester, amide, ether or thioether linkages in the backbone chain; and

R<sub>1</sub> and R<sub>2</sub> each are independently selected unsubstituted alkyl groups having from 1 to about 8 carbon atoms, alkoxyalkyl group having from 2 to about 8 carbon atoms, and substituted alkyl or alkoxyalkyl groups having from 1 to about 8 carbon atoms which are substituted with one or more groups selected from optionally substituted aryl, optionally substituted cycloalkyl, optionally substituted heteroalicyclic, and optionally substituted heteroaryl, wherein at least one of R<sub>1</sub> or R<sub>2</sub> is a substituted alkyl or alkyloxy group;

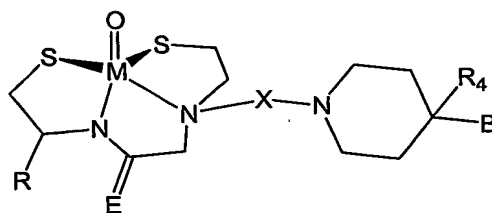
R is selected from hydrogen, C(O)O(R<sub>3</sub>), or C(O)NH(R<sub>3</sub>);

R<sub>3</sub> represents hydrogen, optionally substituted alkyl, optionally substituted alkenyl, optionally substituted alkynyl, optionally substituted aryl, optionally substituted aralkyl, and optionally substituted cycloalkyl; and

E represents an oxo group or two hydrogen atoms.

28. The complex of claim 27, wherein X is an optionally substituted C<sub>2-8</sub>alkylene group, R<sub>1</sub> is C<sub>1-6</sub>alkyl group and R<sub>2</sub> is an optionally substituted (aryl)C<sub>1-4</sub>alkyl or an optionally substituted (heteroaryl)C<sub>1-4</sub>alkyl.

29. The complex of claim 24, wherein the complex is of the formula:



25 wherein

M is one or more isotopes of technetium or rhenium;

B is selected from the group consisting of optionally substituted alkyl, optionally substituted alkenyl, optionally substituted alkynyl, hydroxy, optionally substituted alkoxy, optionally substituted alkoxyalkyl, optionally substituted amino, optionally substituted mono

and dialkyl amino, halogen, optionally substituted aryl, optionally substituted aralkyl, optionally substituted cycloalkyl, optionally substituted heteroalicyclic, optionally substituted heteroaralkyl, optionally substituted heteroaryl, and -X-Y;

R<sub>4</sub> is hydrogen, hydroxy, halogen, optionally substituted alkyl groups having from 1 to about 6 carbon atoms, optionally substituted alkoxy groups having from 1 to about 6 carbon atoms, or

R<sub>4</sub> and B taken in combination form an optionally substituted heterocyclic group having 5 or 12 ring atoms and one or two N, O, or S atoms and 1 or 2 fused rings;

Y is a group capable of chelating to at least one metal ion;

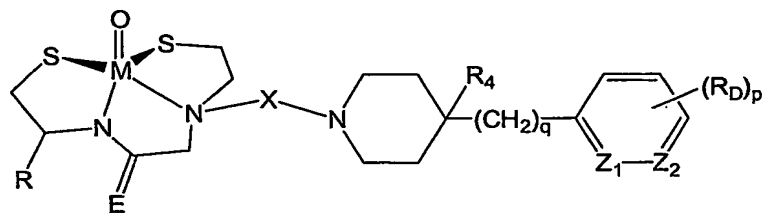
R is selected from hydrogen, C(O)O(R<sub>3</sub>), or C(O)NH(R<sub>3</sub>);

R<sub>3</sub> represents hydrogen, optionally substituted alkyl, optionally substituted alkenyl, optionally substituted alkynyl, optionally substituted aryl, optionally substituted aralkyl, and optionally substituted cycloalkyl;

E represents an oxo group or two hydrogen atoms; and

X is a linking group comprising a backbone chain having 1 to about 8 atoms, the backbone chain can optionally include ester, amide, ether or thioether linkages in the backbone chain.

30. A complex of claim 24, wherein the complex is of the formula:



wherein:

M is one or more isotopes of technetium or rhenium;

R<sub>D</sub> is independently selected at each occurrence from the group consisting of optionally substituted alkyl, optionally substituted alkenyl, optionally substituted alkynyl, hydroxy, amino, halogen, cyano, nitro, optionally substituted alkoxy, optionally substituted alkoxyalkyl, optionally substituted mono and dialkyl amino, optionally substituted aryl, optionally substituted heteroaryl, optionally substituted cycloalkyl, and optionally substituted heteroalicyclic groups;

R<sub>4</sub> is hydrogen, hydroxy, halogen, optionally substituted alkyl groups having from 1 to about 6 carbon atoms, optionally substituted alkoxy groups having from 1 to about 6 carbon atoms;

Z<sub>1</sub> and Z<sub>2</sub> are independently selected from CH, CR<sub>D</sub>, and N;

5 p is selected from integers between about 0 and about 5;

q is selected from integers between about 0 and about 10;

R is selected from hydrogen, C(O)O(R<sub>3</sub>), or C(O)NH(R<sub>3</sub>);

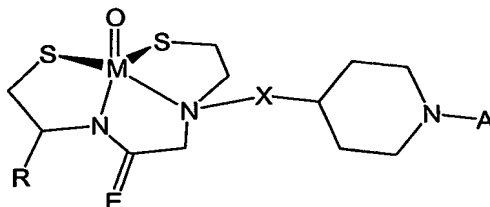
10 R<sub>3</sub> represents hydrogen, optionally substituted alkyl, optionally substituted alkenyl, optionally substituted alkynyl, optionally substituted aryl, optionally substituted aralkyl, and optionally substituted cycloalkyl;

E represents an oxo group or two hydrogen atoms; and

X is a linking group comprising a backbone chain having 1 to about 8 atoms, the backbone chain can optionally include ester, amide, ether or thioether linkages in the backbone chain .

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31. A complex of claim 24, wherein the complex is of the formula:



wherein:

20 M is one or more isotopes of technetium or rhenium;

A is selected from the group consisting of optionally substituted alkyl, optionally substituted alkenyl, optionally substituted alkynyl, optionally substituted aryl, optionally substituted aralkyl, optionally substituted cycloalkyl, optionally substituted heteroalicyclic, optionally substituted heteroaralkyl, optionally substituted heteroaryl, and -X-Y;

25 R is selected from hydrogen, C(O)O(R<sub>3</sub>), or C(O)NH(R<sub>3</sub>);

R<sub>3</sub> represents hydrogen, optionally substituted alkyl, optionally substituted alkenyl, optionally substituted alkynyl, optionally substituted aryl, optionally substituted aralkyl, and optionally substituted cycloalkyl;

E represents an oxo group or two hydrogen atoms; and

X is a linking group comprising a backbone chain having 1 to about 8 atoms, the backbone chain can optionally include ester, amide, ether or thioether linkages in the backbone chain.

5           32.     The complex of any one of claims 24 through 31, wherein the metal ion is radiolabelled or radioactive.

          33.     The complex of any one of claims 24 through 31, wherein the metal ion is not radiolabelled or radioactive.

10

          34.     The complex of any one of claims 24 through 33, wherein the compound is capable of binding to one or more receptors selected from serotonin receptors, adrenergic receptors, adrenoceptors receptors, dopamine receptors, sigma receptors, emopamil binding proteins, calcium channel receptors, or any subtype or subclass thereof.

15

          35.     The complex of claim 34, wherein the receptor(s) e are selected from 5HT<sub>1A</sub>,  $\sigma_1$ ,  $\sigma_2$ ,  $\alpha_1$ , Ca<sup>+2</sup> channel receptor, EBP or a combination thereof.

          36.     A method for in-vivo or in-vitro imaging of at least one tumor comprising the steps of:

20

          providing a radiolabled complex comprising a compound of any one of claims 1-23 and a metal ion or a metal complex of any one of claims 24 through 35;  
          contacting the tumor(s) with the radiolabeled metal complex; and  
          making a radioagraphic image to visualize the tumor(s).

25

          37.     The method of claim 36, wherein the radiolabeled complex comprises a metal ion and a compound of any one of claims 16- 20.

          38.     The method of claim 36, wherein the the metal ion is one or more isotopes of a metal selected from the group consisting of technetium, rhenium, yttrium, copper, gallium, indium, bismuth, platinum and rhodium.

30



39. The method of claim 36, wherein the metal ion is technetium-99m or one or more isotopes of rhenium.

40. The method of claim 36, wherein the tumor(s) are neoplasm(s).

5

41. The method of claim 36, wherein the tumor(s) are carcinoma(s).

42. The method of claim 36, wherein the tumor(s) are melanoma(s).

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43. The method of claim 36, wherein the tumor(s) are prostate carcinoma, breast carcinoma, lung carcinoma, renal carcinoma, colon carcinoma, glioblastoma, neuroblastoma, sarcoma, or a combination thereof.

15 44. The method of any one of claims 36 through 43, wherein the radiolabeled metal complex is capable of binding to one or more proteins or receptors selected from serotonin receptors, adrenergic receptors, adrenoceptors receptors, dopamine receptors, sigma receptors, emopamil binding proteins, calcium channel receptors, or any subtype or subclass thereof.

20 45. The method of claim 44, wherein the protein or receptor(s) are selected from 5HT<sub>1A</sub>,  $\sigma_1$ ,  $\sigma_2$ ,  $\alpha_1$ , Ca<sup>+2</sup> channel receptors, EBP or a combination thereof.

25 46. A method for in-vivo or in-vitro imaging of at least one tissue expressing one or more proteins or receptors for which radiolabeled complexes have affinity, the method comprising the steps of:

providing a radiolabeled complex comprising a compound of any one of claims 1 through 23 and a metal ion or a metal complex of any one of claims 24 through 33;  
contacting the tissue(s) expressing the receptors with the radiolabeled metal complex;  
and  
30 making a radiographic image to visualize the tissue(s).

47. The method of claim 46, wherein the proteins or receptors selected from serotonin receptors, adrenergic receptors, adrenoceptors receptors, dopamine receptors, sigma

receptors, emopamil binding proteins, calcium channel receptors, or any subtype or subclass thereof.

48. The method of claim 46, wherein the protein or receptor expressed by the  
5 tissue to be imaged are selected from 5HT<sub>1A</sub>,  $\sigma_1$ ,  $\sigma_2$ ,  $\alpha_1$ , Ca<sup>2+</sup> channel receptors, EBP or a combination thereof.

49. The method of claim 46, wherein the tissue is part of the central nervous  
10 system or nervous system.

50. The method of claim 49, wherein the tissue is brain tissue expressing the  
protein or receptors.

51. The method of claim 46, wherein the tissue is a tumor.  
15

52. The method of claim 51, wherein the tumor(s) are neoplasm(s), carcinoma(s),  
melanoma(s), or a combination thereof.

53. The method of claim 51, wherein the tumor(s) are melanoma, prostate  
20 carcinoma, breast carcinoma, lung carcinoma, renal carcinoma, colon carcinoma,  
glioblastoma, neuroblastoma, sarcoma, or a combination thereof.

54. A method for the treatment of cancer comprising the steps of:  
providing a cytotoxic metal complex comprising a metal ion and a compound of any  
25 one of claims 1-23 or a metal complex according to any one of claims 24-33; and  
contacting the tumor(s) with the cytotoxic metal complex.

55. The method of claim 56, wherein the cytotoxic metal complex comprises a  
metal ion and a compound of any one of claims 16-20 or a metal complex of any one of  
30 claims 29 through 31 wherein M is one or more isotopes of rhenium.

56. The method of claim 54, wherein the tumor cells express one or more proteins  
or receptors selected from serotonin receptors, adrenergic receptors, adrenoceptors receptors;

dopamine receptors, sigma receptors, emopamil binding proteins, calcium channel receptors, or any subtype or subclass thereof.

57. The method of claim 56, wherein the proteins or receptor are selected from  
5 5HT<sub>1A</sub>,  $\sigma_1$ ,  $\sigma_2$ ,  $\alpha_1$ , Ca<sup>2+</sup> channel receptors, EBP, or a combination thereof.

58. A method of claim 54, wherein the the metal ion is one or more isotopes of a  
metal selected from the group consisting of technetium, rhenium, yttrium, copper, gallium,  
indium, bismuth, platinum, rhodium or a combination thereof.

10

59. The method of claim 54, wherein the tumor(s) are neoplasm(s), carcinoma(s),  
melanoma(s), or a combination thereof.

60. The method of claim 54, wherein the tumor(s) are melanoma, prostate  
15 carcinoma, breast carcinoma, lung carcinoma, renal carcinoma, colon carcinoma,  
glioblastoma, neuroblastoma, sarcoma, or a combination thereof.

20

61. The complex of any one of claims 54 through 60, wherein the metal ion is  
radiolabelled or radioactive.

62. The complex of any one of claims 54 through 60, wherein the metal ion is not  
radiolabelled or radioactive.

63. A method of inhibiting a protein or receptor comprising the steps of:  
25 providing a metal complex comprising a metal ion and a compound of any one of  
claims 1-23 or a metal complex according to any one of claims 24-35; and  
contacting the tumor(s) with the metal complex.

64. The method of claim 63, the protein or receptor are selected from serotonin  
30 receptors, adrenergic receptors, adrenoceptors receptors, dopamine receptors, sigma receptors,  
emopamil binding proteins, calcium channel receptors, or any subtype or subclass thereof.

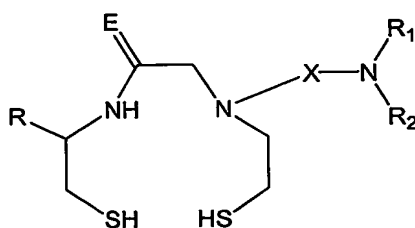
65. The method of claim 63, wherein the neuroreceptor(s) are selected from 5HT<sub>1A</sub>,  $\sigma_1$ ,  $\sigma_2$ ,  $\alpha_1$ , Ca<sup>2+</sup> channel receptors, EBP or a combination thereof.

66. The method of claim 63, wherein the cytotoxic metal complex comprises a metal ion and a compound of any one of claims 16-20 or a metal complex of any one of claims 29 through 31 wherein M is one or more isotopes of rhenium.

67. The complex of any one of claims 63 through 66, wherein the metal ion is radiolabelled or radioactive.

68. The complex of any one of claims 63 through 66, wherein the metal ion is not radiolabelled or radioactive.

69. A compound capable of binding a metal ion, the compound according to the formula:



wherein

X is a linking group comprising a backbone chain having 1 to about 8 atoms, the backbone chain can optionally include ester, amide, ether or thioether linkages in the backbone chain; and

R<sub>1</sub> and R<sub>2</sub> each are independently selected unsubstituted alkyl groups having from 1 to about 8 carbon atoms, alkoxyalkyl group having from 2 to about 8 carbon atoms, and substituted alkyl or alkoxyalkyl groups having from 1 to about 8 carbon atoms which are substituted with one or more groups selected from optionally substituted aryl, optionally substituted cycloalkyl, optionally substituted heteroalicyclic, and optionally substituted heteroaryl, wherein at least one of R<sub>1</sub> or R<sub>2</sub> is a substituted alkyl or alkyloxy group;

R is selected from hydrogen, C(O)O(R<sub>3</sub>), or C(O)NH(R<sub>3</sub>); and

E represents an oxo group or two hydrogen atoms.